

Statistical complexity, Fisher-Shannon information, and Bohr orbits in the H -atom

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Abstract

The Fisher-Shannon information and a statistical measure of complexity are calculated in the position and momentum spaces for the wave functions of the H -atom. For each level of energy, it is found that these two indicators take their minimum values on the orbitals that correspond to the classical (circular) orbits in the Bohr atomic model, just those with the highest orbital angular momentum.

Key words: Statistical Complexity; Fisher-Shannon Information; Hydrogen Atom; Bohr Orbits

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The atom can be considered a complex system. Its structure can be determined through the well established equations of Quantum Mechanics [1,2]. Depending on the set of quantum numbers defining the state of the atom, different conformations are available to it. As a consequence, if the wave function of the atomic state is known, the probability densities in the position and the momentum spaces can be obtained. In this case, the tools that have been developed in information and complexity theories in the last years can be applied [3,4]. Among them, several statistical magnitudes such as Shannon and Fisher informations, different indicators of complexity, etc., can be calculated with a low computational cost [5,6,7,8,9,10,11].

These quantities enlighten new details of the hierarchical organization of the atomic states. In fact, states with the same energy can display, for instance, different values of complexity. Then, it could be interesting to study if the

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hierarchy introduced by these statistical magnitudes could have some physical interpretation. It is our aim to follow this insight. Thus, in this letter, we test this possibility by performing the calculations of some of these magnitudes on the simplest atomic system, that is, the hydrogen atom (*H*-atom).

Let us start by recalling the non-relativistic wave functions of the *H*-atom. These functions in position space ($\vec{r} = (r, \Omega)$, with r the radial distance and Ω the solid angle) are:

$$\Psi_{n,l,m}(\vec{r}) = R_{n,l}(r) Y_{l,m}(\Omega) , \quad (1)$$

where $R_{n,l}(r)$ is the radial part and $Y_{l,m}(\Omega)$ is the spherical harmonic of the atomic state determined by the quantum numbers (n, l, m) . The radial part is expressed as [2]

$$R_{n,l}(r) = \frac{2}{n^2} \left[\frac{(n-l-1)!}{(n+l)!} \right]^{1/2} \left(\frac{2r}{n} \right)^l e^{-\frac{r}{n}} L_{n-l-1}^{2l+1} \left(\frac{2r}{n} \right) , \quad (2)$$

being $L_\alpha^\beta(t)$ the associated Laguerre polynomials. Atomic units are used through the text.

The same functions in momentum space ($\vec{p} = (p, \hat{\Omega})$, with p the momentum modulus and $\hat{\Omega}$ the solid angle) are:

$$\hat{\Psi}_{n,l,m}(\vec{p}) = \hat{R}_{n,l}(p) Y_{l,m}(\hat{\Omega}) , \quad (3)$$

where the radial part $\hat{R}_{n,l}(p)$ is now given by the expression [12]

$$\hat{R}_{n,l}(p) = \left[\frac{2}{\pi} \frac{(n-l-1)!}{(n+l)!} \right]^{1/2} n^2 2^{2l+2} l! \frac{n^l p^l}{(n^2 p^2 + 1)^{l+2}} C_{n-l-1}^{l+1} \left(\frac{n^2 p^2 - 1}{n^2 p^2 + 1} \right) , \quad (4)$$

with $C_\alpha^\beta(t)$ the Gegenbauer polynomials.

Taking the former expressions, the probability density in position and momentum spaces,

$$\rho(\vec{r}) = |\Psi_{n,l,m}(\vec{r})|^2 , \quad \gamma(\vec{p}) = |\hat{\Psi}_{n,l,m}(\vec{p})|^2 , \quad (5)$$

can be explicitly calculated. From these densities, we proceed now to compute the statistical complexity and the Fisher-Shannon information.

First, the measure of complexity C recently introduced by Lopez-Ruiz, Mancini and Calbet [13,14,15,16], the so-called *LMC* complexity, is defined as

$$C = H \cdot D , \quad (6)$$

where H represents the information content of the system and D is the distance from the actual state of the system to some prestablished reference state.

For our purpose, we take a version used in Ref. [15] as quantifier of H . This is the simple exponential Shannon entropy, that in the position and momentum spaces takes the form, respectively,

$$H_r = e^{S_r}, \quad H_p = e^{S_p}. \quad (7)$$

S_r and S_p are the Shannon information entropies [17],

$$S_r = - \int \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r}, \quad S_p = - \int \gamma(\vec{p}) \log \gamma(\vec{p}) d\vec{p}. \quad (8)$$

We keep for the disequilibrium the form originally introduced in Refs. [13,15], that is,

$$D_r = \int \rho^2(\vec{r}) d\vec{r}, \quad D_p = \int \gamma^2(\vec{p}) d\vec{p}, \quad (9)$$

In this manner, the final expressions for C in position and momentum spaces are:

$$C_r = H_r \cdot D_r, \quad C_p = H_p \cdot D_p. \quad (10)$$

These quantities are plotted in Fig. 1 as function of the modulus of the third component m of the orbital angular momentum l for different pairs of (n, l) values. Let us recall at this point the range of the quantum numbers: $n \geq 1$, $0 \leq l \leq n - 1$, and $-l \leq m \leq l$. Fig. 1(a) shows C_r for $n = 15$ and Fig. 1(b) shows C_r for $n = 30$. In both figures, it can be observed that C_r splits in different sets of discrete points. Each one of these sets is associated to a different l value. It is worth to note that the set with the minimum values of C_r corresponds just to the highest l , that is, $l = n - 1$. The same behavior can be observed in Figs. 1(c) and 1(d) for C_p .

Second, other types of statistical measures that maintain the product form of C can be defined. Let us take, for instance, the Fisher-Shannon P information that has been also applied in Refs. [7,11] in atomic systems. This quantity, in the position and momentum spaces, is given respectively by

$$P_r = J_r \cdot I_r, \quad P_p = J_p \cdot I_p, \quad (11)$$

where the first factor

$$J_r = \frac{1}{2\pi e} e^{2S_r/3}, \quad J_p = \frac{1}{2\pi e} e^{2S_p/3}, \quad (12)$$

is a version of the exponential Shannon entropy [18], and the second factor

$$I_r = \int \frac{[\vec{\nabla} \rho(\vec{r})]^2}{\rho(\vec{r})} d\vec{r}, \quad I_p = \int \frac{[\vec{\nabla} \gamma(\vec{p})]^2}{\gamma(\vec{p})} d\vec{p}, \quad (13)$$

is the so-called Fisher information measure [19], that quantifies the narrowness of the probability density. This last indicator can be analytically obtained in

both spaces (position and momentum). The results are [8]:

$$I_r = \frac{4}{n^2} \left(1 - \frac{|m|}{n} \right), \quad (14)$$

$$I_p = 2n^2 \left\{ 5n^2 + 1 - 3l(l+1) - (8n - 3(2l+1)) |m| \right\}. \quad (15)$$

Fig. 2 shows the calculation of P as function of the modulus of the third component m for different pairs of (n, l) values. In Fig. 2(a), P_r is plotted for $n = 15$, and P_r is plotted for $n = 30$ in Fig. 2(b). Here P_r also splits in different sets of discrete points, showing a behavior parallel to the above signaled for C (Fig. 1). Each one of these sets is also related with a different l value. We remark again that the set with the minimum values of P_r corresponds just to the highest l . In Figs. 2(c) and 2(d), the same behavior can be observed for P_p .

Let us finish this short note with the conclusions. The statistical complexity and the Fisher-Shannon information have been computed on the H -atom. In this case, we have taken advantage of the exact knowledge of the wave functions. Concretely, we put in evidence that, for a fixed level of energy n , these statistical magnitudes take their minimum values for the highest allowed orbital angular momentum, $l = n - 1$. It is worth to remember at this point that the radial part of this particular wave function, that describes the electron in the $(n, l = n - 1)$ orbital, has no nodes. This means that the spatial configuration of this atomic state is, in some way, a spherical-like shell. In fact, the mean radius of this shell, $\langle r \rangle_{n,l,m}$, which is given by [20]

$$\langle r \rangle_{n,l=n-1,m} \equiv \langle r \rangle_{n,l=n-1} = n^2 \left(1 + \frac{1}{2n} \right), \quad (16)$$

tends, when $n \gg 1$, to the radius of the n th energy level, $r_{Bohr} = n^2$, of the Bohr atom.

It is remarkable that the minimum values of these statistical measures calculated from the quantum wave functions of the H -atom enhance our intuition by selecting just those orbitals that in the pre-quantum image are the Bohr orbits. Therefore, we conclude that the results here reported show that new insights could be inferred from these magnitudes at the quantum level.

References

- [1] L.D. Landau and L.M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory*, Volume 3, Third Edition, Butterworth-Heinemann, Oxford, 1981.
- [2] A. Galindo and P. Pascual, *Quantum Mechanics I*, Springer, Berlin, 1991.

- [3] S.R. Gadre and R.D. Bendale, Phys. Rev. A **36** (1987) 1932.
- [4] K.Ch. Chatzisavvas, Ch.C. Moustakidis, and C.P. Panos, J. Chem. Phys. **123** (2005) 174111.
- [5] S.R. Gadre, S.B. Sears, S.J. Chakravorty, and R.D. Bendale, Phys. Rev. A **32** (1985) 2602.
- [6] R.J. Yanez, W. van Assche, and J.S. Dehesa, Phys. Rev. A 50 (1994) 3065.
- [7] E. Romera and J.S. Dehesa, J. Chem. Phys. 120 (2004) 8906.
- [8] E. Romera, P. Sanchez-Moreno, and J.S. Dehesa, Chem. Phys. Lett. **414** (2005) 468.
- [9] C.P. Panos, K.Ch. Chatzisavvas, Ch.C. Moustakidis, and E.G. Kyrkou, Phys. Lett. A **363** (2007) 78.
- [10] S.H. Patil, K.D. Sen, N.A. Watson, and H.E. Montgomery Jr., J. Phys. B: At. Mol. Opt. Phys. **40** (2007) 2147.
- [11] H.E. Montgomery Jr. and K.D. Sen, Phys. Lett. A, in press (2007) doi:10.1016/j.physleta.2007.11.041.
- [12] H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of One-And Two-Electron Atoms*, Springer, Berlin, 1977.
- [13] R. Lopez-Ruiz, H.L. Mancini, and X. Calbet, Phys. lett. A **209** (1995) 321.
- [14] X. Calbet and R. Lopez-Ruiz, Phys. Rev. E **63** (2001) 066116.
- [15] R.G. Catalan, J. Garay, and R. Lopez-Ruiz, Phys. Rev. E **66** (2002) 011102.
- [16] R. Lopez-Ruiz, Biophys. Chem. **115** (2005) 215.
- [17] C.E. Shannon, *A mathematical theory of communication*, Bell. Sys. Tech. J. **27** (1948) 379; ibid. (1948) 623.
- [18] A. Dembo, T.A. Cover, and J.A. Thomas, IEEE Trans. Inf. Theory 37 (1991) 1501.
- [19] R.A. Fisher, Proc. Cambridge Phil. Sec. **22** (1925) 700.
- [20] J.L. Eisberg, *Fundamentals of Modern Physics*, J. Wiley & Sons, New York, 1961.

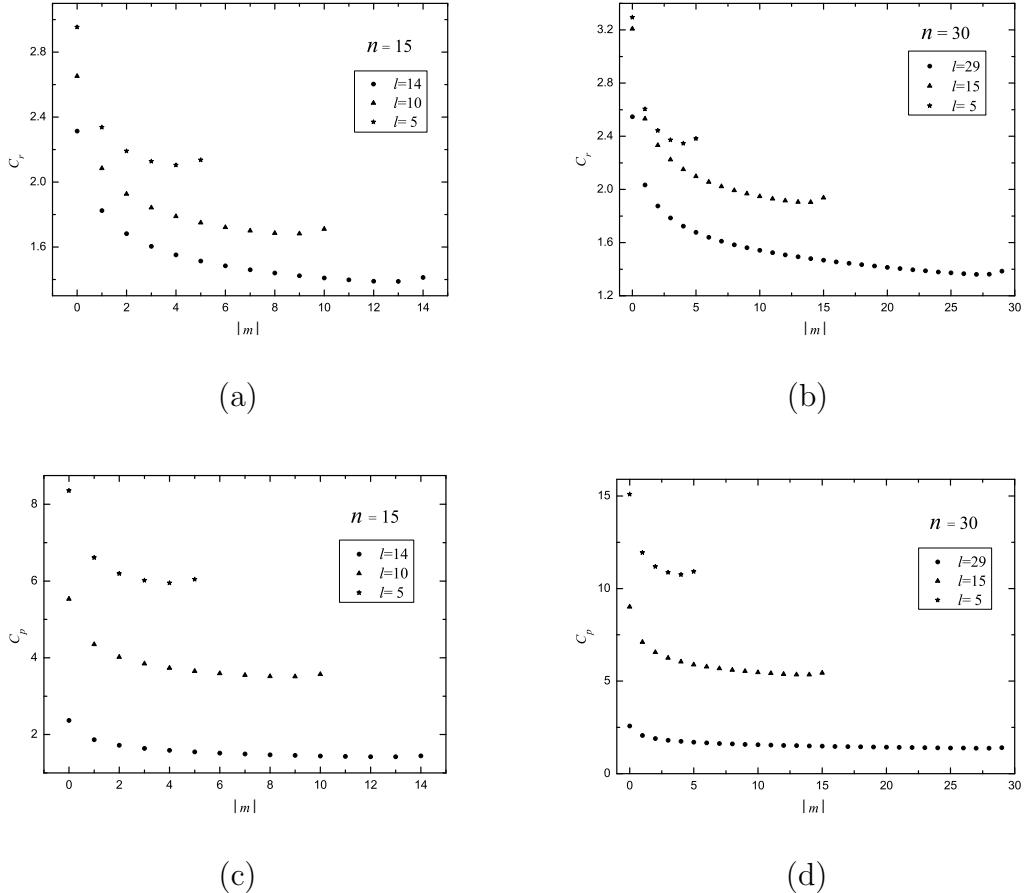


Fig. 1. Statistical complexity in position space, C_r , and momentum space, C_p , vs. $|m|$ for different (n, l) values in the hydrogen atom. C_r for (a) $n = 15$ and (b) $n = 30$. C_p for (c) $n = 15$ and (d) $n = 30$. All values are in atomic units.

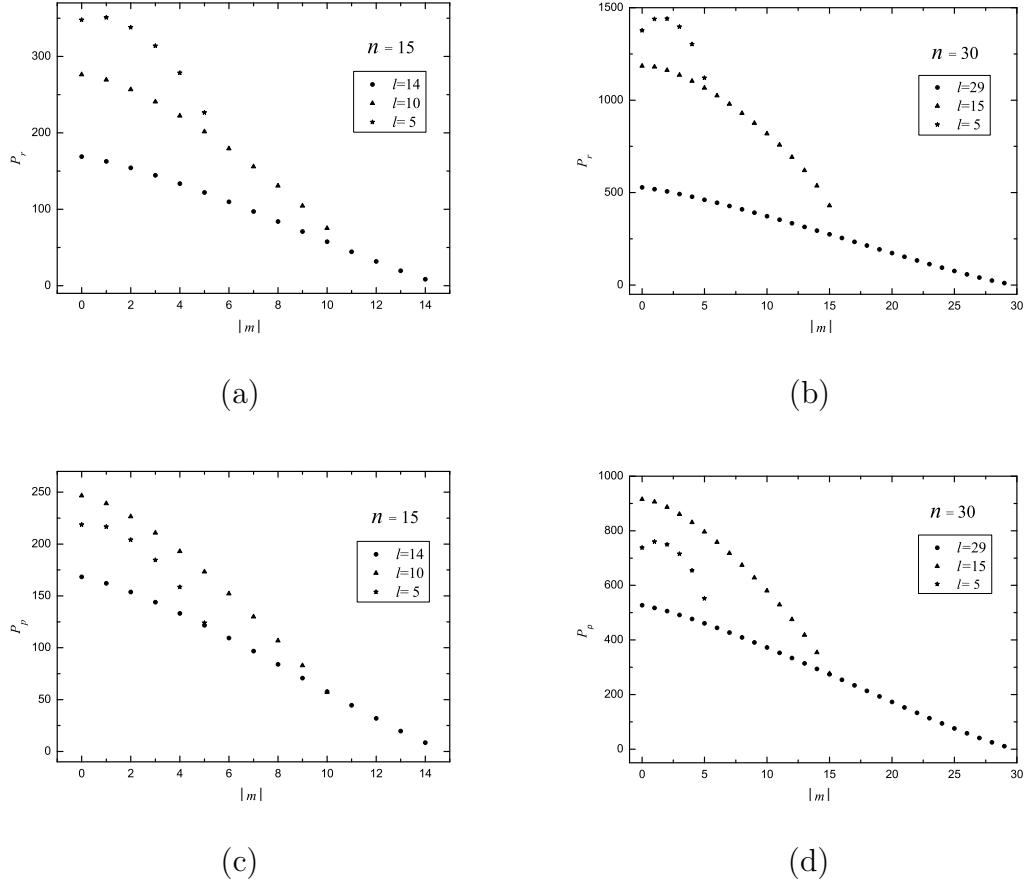


Fig. 2. Fisher-Shannon information in position space, P_r , and momentum space, P_p , vs. $|m|$ for different (n, l) values in the hydrogen atom. P_r for (a) $n = 15$ and (b) $n = 30$. P_p for (c) $n = 15$ and (d) $n = 30$. All values are in atomic units.